

Tore Brinck

List of Publications by Year in descending order

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142
papers

9,289
citations

47409

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160
docs citations

160
times ranked

8711
citing authors

#	ARTICLE	IF	CITATIONS
1	Machine learning meets mechanistic modelling for accurate prediction of experimental activation energies. <i>Chemical Science</i> , 2021, 12, 1163-1175.	3.7	102
2	Improving the Stability of Trinitramide by Chemical Substitution: N(NF ₂) ₃ has Higher Stability and Excellent Propulsion Performance. <i>Propellants, Explosives, Pyrotechnics</i> , 2021, 46, 245-252.	1.0	4
3	Acetic acid conversion to ketene on Cu ₂ O(1 0 0): Reaction mechanism deduced from experimental observations and theoretical computations. <i>Journal of Catalysis</i> , 2021, 402, 154-165.	3.1	3
4	Utilizing the Surface Electrostatic Potential to Predict the Interactions of Pt and Ni Nanoparticles with Lewis Acids and Bases— Γ -Lumps and Γ -Holes Govern the Catalytic Activities. <i>Journal of Physical Chemistry C</i> , 2020, 124, 14696-14705.	1.5	13
5	The Surface Structure of Cu ₂ O(100): Nature of Defects. <i>Journal of Physical Chemistry C</i> , 2019, 123, 7696-7704.	1.5	13
6	The local electron attachment energy and the electrostatic potential as descriptors of surface-adsorbate interactions. <i>Physical Chemistry Chemical Physics</i> , 2019, 21, 17001-17009.	1.3	10
7	Asymmetric Synthesis of Adjacent Tri- and Tetrasubstituted Carbon Stereocenters: Organocatalytic Aldol Reaction of an Hydantoin Surrogate with Azaarene α -Carbaldehydes. <i>Chemistry - A European Journal</i> , 2019, 25, 12431-12438.	1.7	15
8	Interaction of Atomic Hydrogen with the Cu ₂ O(100) and (111) Surfaces. <i>Journal of Physical Chemistry C</i> , 2019, 123, 22172-22180.	1.5	13
9	Electrostatics and polarization determine the strength of the halogen bond: a red card for charge transfer. <i>Journal of Molecular Modeling</i> , 2019, 25, 125.	0.8	42
10	The Molecular Surface Property Approach: A Guide to Chemical Interactions in Chemistry, Medicine, and Material Science. <i>Advanced Theory and Simulations</i> , 2019, 2, 1800149.	1.3	36
11	Chemical Reactivity: The Molecular Surface Property Approach: A Guide to Chemical Interactions in Chemistry, Medicine, and Material Science (Adv. Theory Simul. 1/2019). <i>Advanced Theory and Simulations</i> , 2019, 2, 1970003.	1.3	1
12	Theoretical Investigation into Rate-Determining Factors in Electrophilic Aromatic Halogenation. <i>Journal of Physical Chemistry A</i> , 2018, 122, 3270-3279.	1.1	22
13	Mechanism and regioselectivity of electrophilic aromatic nitration in solution: the validity of the transition state approach. <i>Journal of Molecular Modeling</i> , 2018, 24, 15.	0.8	29
14	Γ -Holes and Γ -lumps direct the Lewis basic and acidic interactions of noble metal nanoparticles: introducing regium bonds. <i>Physical Chemistry Chemical Physics</i> , 2018, 20, 2676-2692.	1.3	99
15	Nucleophilic Aromatic Substitution Reactions Described by the Local Electron Attachment Energy. <i>Journal of Organic Chemistry</i> , 2017, 82, 3072-3083.	1.7	38
16	Interaction of Sulfur Dioxide and Near-Ambient Pressures of Water Vapor with Cuprous Oxide Surfaces. <i>Journal of Physical Chemistry C</i> , 2017, 121, 24011-24024.	1.5	11
17	On the Kinetic and Thermodynamic Properties of Aryl Radicals Using Electrochemical and Theoretical Approaches. <i>ChemElectroChem</i> , 2017, 4, 3212-3221.	1.7	12
18	Computational analysis of the early stage of cuprous oxide sulphidation: a top-down process. <i>Corrosion Engineering Science and Technology</i> , 2017, 52, 50-53.	0.7	13

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19	Extending the σ -Hole Concept to Metals: An Electrostatic Interpretation of the Effects of Nanostructure in Gold and Platinum Catalysis. <i>Journal of the American Chemical Society</i> , 2017, 139, 11012-11015.	6.6	136
20	MD Simulations Reveal Complex Water Paths in Squalene-Hopene Cyclase: Tunnel-Obstructing Mutations Increase the Flow of Water in the Active Site. <i>ACS Omega</i> , 2017, 2, 8495-8506.	1.6	6
21	Local Lewis Acidity of $(\text{TiO}_2)_n$ ($n = 7-10$) Nanoparticles Characterized by DFT-Based Descriptors: Tools for Catalyst Design. <i>Journal of Physical Chemistry C</i> , 2017, 121, 27483-27492.	1.5	14
22	Dehydrogenation of methanol on $\text{Cu}_2\text{O}(100)$ and (111). <i>Journal of Chemical Physics</i> , 2017, 146, 244702.	1.2	23
23	σ -Holes on Transition Metal Nanoclusters and Their Influence on the Local Lewis Acidity. <i>Crystals</i> , 2017, 7, 222.	1.0	16
24	Local Electron Attachment Energy and Its Use for Predicting Nucleophilic Reactions and Halogen Bonding. <i>Journal of Physical Chemistry A</i> , 2016, 120, 10023-10032.	1.1	27
25	Fragment molecular orbital study of the cAMP-dependent protein kinase catalyzed phosphoryl transfer: a comparison with the differential transition state stabilization method. <i>Physical Chemistry Chemical Physics</i> , 2016, 18, 15153-15161.	1.3	5
26	Reactivity at the $\text{Cu}_2\text{O}(100):\text{Cu-H}_2\text{O}$ interface: a combined DFT and PES study. <i>Physical Chemistry Chemical Physics</i> , 2016, 18, 30570-30584.	1.3	21
27	Aqueous Solvation and Surface Oxidation of the Cu_7 Nanoparticle: Insights from Theoretical Modeling. <i>Journal of Physical Chemistry C</i> , 2016, 120, 1977-1988.	1.5	12
28	Surface Reactions of H_2O_2 , H_2 , and O_2 in Aqueous Systems Containing ZrO_2 . <i>Journal of Physical Chemistry C</i> , 2016, 120, 1609-1614.	1.5	16
29	Dual Lewis Acid/Lewis Base Catalyzed Acylcyanation of Aldehydes: A Mechanistic Study. <i>Chemistry - A European Journal</i> , 2016, 22, 3821-3829.	1.7	9
30	The Surface Structure of $\text{Cu}_2\text{O}(100)$. <i>Journal of Physical Chemistry C</i> , 2016, 120, 4373-4381.	1.5	46
31	Application of reactivity descriptors to the catalytic decomposition of hydrogen peroxide at oxide surfaces. <i>Computational and Theoretical Chemistry</i> , 2015, 1070, 108-116.	1.1	18
32	Novel Approach for Identifying Key Residues in Enzymatic Reactions: Proton Abstraction in Ketosteroid Isomerase. <i>Journal of Physical Chemistry B</i> , 2014, 118, 13050-13058.	1.2	14
33	Binder Materials for Green Propellants. , 2014, , 205-234.		3
34	Some Perspectives on Sensitivity to Initiation of Detonation. , 2014, , 45-62.		20
35	Searching for the thermodynamic limit - a DFT study of the step-wise water oxidation of the bipyramidal Cu_7 cluster. <i>Physical Chemistry Chemical Physics</i> , 2014, 16, 2452-2464.	1.3	24
36	Ionization of ammonium dinitramide: decomposition pathways and ionization products. <i>Theoretical Chemistry Accounts</i> , 2013, 132, 1.	0.5	9

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37	Reactivity of metal oxide clusters with hydrogen peroxide and water – a DFT study evaluating the performance of different exchange–correlation functionals. <i>Physical Chemistry Chemical Physics</i> , 2013, 15, 5539.	1.3	73
38	In situ confocal Raman micro-spectroscopy and electrochemical studies of mussel adhesive protein and ceria composite film on carbon steel in salt solutions. <i>Electrochimica Acta</i> , 2013, 107, 276-291.	2.6	31
39	On the method-dependence of transition state asynchronicity in Diels–Alder reactions. <i>Physical Chemistry Chemical Physics</i> , 2013, 15, 5108.	1.3	76
40	Control of the ambident reactivity of the nitrite ion. <i>Organic and Biomolecular Chemistry</i> , 2013, 11, 648-653.	1.5	33
41	In situ investigations of Fe ³⁺ induced complexation of adsorbed Mefp-1 protein film on iron substrate. <i>Journal of Colloid and Interface Science</i> , 2013, 404, 62-71.	5.0	28
42	Utilizing the π -complex stability for quantifying reactivity in nucleophilic substitution of aromatic fluorides. <i>Beilstein Journal of Organic Chemistry</i> , 2013, 9, 791-799.	1.3	19
43	–Adapted Linear Interaction Energy– A Structure-Based LIE Parametrization for Fast Prediction of Protein–Ligand Affinities. <i>Journal of Chemical Theory and Computation</i> , 2013, 9, 1230-1239.	2.3	5
44	Mechanism of H ₂ O ₂ Decomposition on Transition Metal Oxide Surfaces. <i>Journal of Physical Chemistry C</i> , 2012, 116, 9533-9543.	1.5	223
45	Envisioning an enzymatic Diels–Alder reaction by in situ acid–base catalyzed diene generation. <i>Chemical Communications</i> , 2012, 48, 5665.	2.2	12
46	Computational design of a Diels–Alderase from a thermophilic esterase: the importance of dynamics. <i>Journal of Computer-Aided Molecular Design</i> , 2012, 26, 1079-1095.	1.3	12
47	Mechanistic Insights into the Stepwise Diels–Alder Reaction of 4,6-Dinitrobenzofuroxan. <i>Organic Letters</i> , 2012, 14, 118-121.	2.4	26
48	Electrochemical, atomic force microscopy and infrared reflection absorption spectroscopy studies of pre-formed mussel adhesive protein films on carbon steel for corrosion protection. <i>Thin Solid Films</i> , 2012, 520, 7136-7143.	0.8	18
49	Predicting Regioselectivity in Nucleophilic Aromatic Substitution. <i>Journal of Organic Chemistry</i> , 2012, 77, 3262-3269.	1.7	37
50	Stepwise Diels–Alder: More than Just an Oddity? A Computational Mechanistic Study. <i>Journal of Organic Chemistry</i> , 2012, 77, 6563-6573.	1.7	52
51	The Molecular Surface Structure of Ammonium and Potassium Dinitramide: A Vibrational Sum Frequency Spectroscopy and Quantum Chemical Study. <i>Journal of Physical Chemistry C</i> , 2011, 115, 10588-10596.	1.5	7
52	Designing a New Diels–Alderase: A Combinatorial, Semirational Approach Including Dynamic Optimization.. <i>Journal of Chemical Information and Modeling</i> , 2011, 51, 1906-1917.	2.5	11
53	Computational design of a lipase for catalysis of the Diels-Alder reaction. <i>Journal of Molecular Modeling</i> , 2011, 17, 833-849.	0.8	12
54	Experimental Detection of Trinitramide, N(NO ₂) ₃ . <i>Angewandte Chemie - International Edition</i> , 2011, 50, 1145-1148.	7.2	38

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55	Racemase Activity of <i>B. cepacia</i> Lipase Leads to Dual-Function Asymmetric Dynamic Kinetic Resolution of β -Aminonitriles. <i>Angewandte Chemie - International Edition</i> , 2011, 50, 6592-6595.	7.2	37
56	A pragmatic procedure for predicting regioselectivity in nucleophilic substitution of aromatic fluorides. <i>Tetrahedron Letters</i> , 2011, 52, 3150-3153.	0.7	18
57	On the formation of hydrogen gas on copper in anoxic water. <i>Journal of Chemical Physics</i> , 2011, 135, 084709.	1.2	24
58	Validation of a Computational Model for Predicting the Site for Electrophilic Substitution in Aromatic Systems. <i>Journal of Organic Chemistry</i> , 2010, 75, 4696-4705.	1.7	42
59	Generation of soluble oligomeric β -amyloid species via copper catalyzed oxidation with implications for Alzheimer's disease: A DFT study. <i>Journal of Molecular Modeling</i> , 2010, 16, 1103-1108.	0.8	5
60	Quantitative analysis of molecular surfaces: areas, volumes, electrostatic potentials and average local ionization energies. <i>Journal of Molecular Modeling</i> , 2010, 16, 1679-1691.	0.8	985
61	Kinetic Stability and Propellant Performance of Green Energetic Materials. <i>Chemistry - A European Journal</i> , 2010, 16, 6590-6600.	1.7	69
62	Diastereoselective One-Pot Tandem Synthesis of 3-Substituted Isoindolinones: A Mechanistic Investigation. <i>Journal of Organic Chemistry</i> , 2010, 75, 5882-5887.	1.7	38
63	On the Anomalous Decomposition and Reactivity of Ammonium and Potassium Dinitramide. <i>Journal of Physical Chemistry A</i> , 2010, 114, 2845-2854.	1.1	36
64	Synthesis and Mechanistic Studies of Organic Chromophores with Different Energy Levels for p-Type Dye-Sensitized Solar Cells. <i>Journal of Physical Chemistry C</i> , 2010, 114, 4738-4748.	1.5	174
65	pH-Dependent Mutarotation of 1-Thioaldoses in Water. Unexpected Behavior of (2S)-d-Aldopyranoses. <i>Journal of Organic Chemistry</i> , 2010, 75, 6115-6121.	1.7	27
66	High Incident Photon-to-Current Conversion Efficiency of p-Type Dye-Sensitized Solar Cells Based on NiO and Organic Chromophores. <i>Advanced Materials</i> , 2009, 21, 2993-2996.	11.1	173
67	Rhodanine dyes for dye-sensitized solar cells: spectroscopy, energy levels and photovoltaic performance. <i>Physical Chemistry Chemical Physics</i> , 2009, 11, 133-141.	1.3	178
68	Symmetric and unsymmetric donor functionalization. comparing structural and spectral benefits of chromophores for dye-sensitized solar cells. <i>Journal of Materials Chemistry</i> , 2009, 19, 7232.	6.7	177
69	Molecular dynamics study of zinc binding to cysteines in a peptide mimic of the alcohol dehydrogenase structural zinc site. <i>Physical Chemistry Chemical Physics</i> , 2009, 11, 975-983.	1.3	54
70	The anomalous solid state decomposition of ammonium dinitramide: a matter of surface polarization. <i>Chemical Communications</i> , 2009, , 2896.	2.2	14
71	Synergistic activation of the Diels-Alder reaction by an organic catalyst and substituents: a computational study. <i>Organic and Biomolecular Chemistry</i> , 2009, 7, 1304.	1.5	18
72	Direct Epoxidation in <i>Candida antarctica</i> Lipase B Studied by Experiment and Theory. <i>ChemBioChem</i> , 2008, 9, 2443-2451.	1.3	78

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73	HCCI experiments with toluene reference fuels modeled by a semidetailed chemical kinetic model. <i>Combustion and Flame</i> , 2008, 155, 696-712.	2.8	195
74	Dinitraminic acid (HDN) isomerization and self-decomposition revisited. <i>Chemical Physics</i> , 2008, 348, 53-60.	0.9	17
75	Phosphine-catalyzed disulfide metathesis. <i>Chemical Communications</i> , 2008, , 6603.	2.2	85
76	Novel 1,3-Dipolar Cycloadditions of Dinitraminic Acid: Implications for the Chemical Stability of Ammonium Dinitramide. <i>Journal of Physical Chemistry A</i> , 2008, 112, 2456-2463.	1.1	17
77	Supramolecular Control in Carbohydrate Epimerization: Discovery of a New Anion Host-Guest System. <i>Journal of the American Chemical Society</i> , 2008, 130, 15270-15271.	6.6	26
78	Tuning the HOMO and LUMO Energy Levels of Organic Chromophores for Dye Sensitized Solar Cells. <i>Journal of Organic Chemistry</i> , 2007, 72, 9550-9556.	1.7	576
79	A combined molecular dynamics simulation and quantum chemical study on the mechanism for activation of the OxyR transcription factor by hydrogen peroxide. <i>Organic and Biomolecular Chemistry</i> , 2006, 4, 3468-3478.	1.5	18
80	Electrostatic potential as a measure of gas phase carbocation stability. <i>International Journal of Quantum Chemistry</i> , 2006, 106, 2904-2909.	1.0	15
81	Exploring the Active-Site of a Rationally Redesigned Lipase for Catalysis of Michael-Type Additions. <i>ChemBioChem</i> , 2005, 6, 331-336.	1.3	135
82	Elucidation of the Thermochemical Properties of Triphenyl- or Tributyl-Substituted Si-, Ge-, and Sn-Centered Radicals by Means of Electrochemical Approaches and Computations. <i>Journal of the American Chemical Society</i> , 2005, 127, 2677-2685.	6.6	22
83	Aldol additions with mutant lipase: analysis by experiments and theoretical calculations. <i>Journal of Molecular Catalysis B: Enzymatic</i> , 2004, 31, 123-128.	1.8	65
84	Thiol-ene coupling reaction of fatty acid monomers. <i>Journal of Polymer Science Part A</i> , 2004, 42, 6346-6352.	2.5	74
85	Polymer-assisted laser desorption/ionization analysis of small molecular weight compounds. <i>Rapid Communications in Mass Spectrometry</i> , 2004, 18, 841-852.	0.7	34
86	Computation of Franck-Condon factors for many-atom systems: simulated photoelectron spectra of formic acid isotopologues. <i>Chemical Physics</i> , 2004, 302, 217-228.	0.9	6
87	The Stability of Arylpentazoles. <i>Journal of Physical Chemistry A</i> , 2004, 108, 7463-7467.	1.1	58
88	Computational Study of the Amination of Halobenzenes and Phenylpentazole. A Viable Route to Isolate the Pentazolate Anion?. <i>Journal of Organic Chemistry</i> , 2004, 69, 3222-3225.	1.7	14
89	Carbon-Carbon Bonds by Hydrolytic Enzymes. <i>Journal of the American Chemical Society</i> , 2003, 125, 874-875.	6.6	249
90	Segmental analysis of molecular surface electrostatic potentials: application to enzyme inhibition. <i>Journal of Molecular Modeling</i> , 2003, 9, 77-83.	0.8	20

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91	Rational design of a lipase to accommodate catalysis of Baeyer-Villiger oxidation with hydrogen peroxide. <i>Journal of Molecular Modeling</i> , 2003, 9, 164-171.	0.8	34
92	Detection of pentazolone anion (cyclo-N ₅ ⁺) from laser ionization and decomposition of solid p-dimethylaminophenylpentazole. <i>Chemical Physics Letters</i> , 2003, 379, 539-546.	1.2	114
93	Computational prediction of relative group polarizabilities. <i>International Journal of Quantum Chemistry</i> , 2003, 95, 632-637.	1.0	19
94	Thermochemistry of Arylselenyl Radicals and the Pertinent Ions in Acetonitrile. <i>Journal of the American Chemical Society</i> , 2003, 125, 2148-2157.	6.6	27
95	Reaction of Peroxyl Radicals with Ozone in Water. <i>Journal of Physical Chemistry A</i> , 2003, 107, 676-681.	1.1	25
96	Electronic structure calculations as a tool in the quest for experimental verification of N ₄ . <i>Theoretical and Computational Chemistry</i> , 2003, , 421-439.	0.2	6
97	Solvation of Sulfur-Centered Cations and Anions in Acetonitrile. <i>Journal of Physical Chemistry A</i> , 2002, 106, 8827-8833.	1.1	23
98	Prediction of Solubility of Solid Organic Compounds in Solvents by UNIFAC. <i>Industrial & Engineering Chemistry Research</i> , 2002, 41, 5114-5124.	1.8	98
99	A theoretical study of the azide (N ₃) doublet states. A new route to tetraazetetrahedrane (N ₄): N+N ₃ ⁺ N ₄ . <i>Journal of Chemical Physics</i> , 2002, 116, 9740-9748.	1.2	50
100	A Theoretical Study of the Uncatalyzed and BF ₃ -Assisted Baeyer-Villiger Reactions. <i>Journal of Organic Chemistry</i> , 2001, 66, 1193-1199.	1.7	53
101	How Does Methylithium Invert? A Density Functional Study. <i>Organometallics</i> , 2001, 20, 5134-5138.	1.1	10
102	Ab initio study of the ground state and the first excited state of the rectangular (D _{2h})N ₄ molecule. <i>Chemical Physics Letters</i> , 2001, 347, 220-228.	1.2	26
103	Theoretical study of the singlet electronically excited states of N ₄ . <i>Chemical Physics Letters</i> , 2001, 340, 597-603.	1.2	23
104	Theoretical Study of the Triplet N ₄ Potential Energy Surface. <i>Journal of Physical Chemistry A</i> , 2000, 104, 11999-12005.	1.1	45
105	Solvation of Carbanions in Organic Solvents: A Test of the Polarizable Continuum Model. <i>Journal of Physical Chemistry B</i> , 2000, 104, 9887-9893.	1.2	24
106	Two potential energetic compounds: Ammonium superoxide and ammonium ozonide. <i>Journal of Energetic Materials</i> , 2000, 18, 89-95.	1.0	1
107	The catalytic effect of water in basic hydrolysis of methyl acetate: a theoretical study. <i>Computational and Theoretical Chemistry</i> , 1999, 459, 85-93.	1.5	34
108	Quantum Chemical Studies on the Thermochemistry of Alkyl and Peroxyl Radicals. <i>Journal of Physical Chemistry A</i> , 1999, 103, 7094-7104.	1.1	65

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109	Theoretical Studies of the Hydrolysis of the Methyl Phosphate Anion. <i>Journal of Physical Chemistry A</i> , 1999, 103, 5379-5386.	1.1	100
110	Ab initio and density functional theory studies of the catalytic mechanism for ester hydrolysis in serine hydrolases. <i>International Journal of Quantum Chemistry</i> , 1998, 69, 89-103.	1.0	54
111	The use of the electrostatic potential for analysis and prediction of intermolecular interactions. <i>Theoretical and Computational Chemistry</i> , 1998, , 51-93.	0.2	21
112	Modified Interaction Properties Function for the Analysis and Prediction of Lewis Basicities. <i>Journal of Physical Chemistry A</i> , 1997, 101, 3408-3415.	1.1	18
113	A Computational Analysis of Substituent Effects on the O-H Bond Dissociation Energy in Phenols: Polar Versus Radical Effects. <i>Journal of the American Chemical Society</i> , 1997, 119, 4239-4244.	6.6	170
114	Prediction of water-octanol partition coefficients using theoretical descriptors derived from the molecular surface area and the electrostatic potential. <i>Journal of the Chemical Society Perkin Transactions II</i> , 1997, , 289-294.	0.9	42
115	Force field parameterization of copper(I)-olefin systems from density functional calculations. <i>Computational and Theoretical Chemistry</i> , 1997, 397, 39-50.	1.5	19
116	Computational Analysis of Substituent Effects in Para-Substituted Phenoxide Ions. <i>The Journal of Physical Chemistry</i> , 1996, 100, 10116-10120.	2.9	30
117	Relationships of molecular surface electrostatic potentials to some macroscopic properties. <i>Chemical Physics</i> , 1996, 204, 289-299.	0.9	85
118	Analytical Representation and Prediction of Macroscopic Properties. <i>ACS Symposium Series</i> , 1995, , 109-118.	0.5	6
119	Family-independent relationships between computed molecular surface quantities and solute hydrogen bond acidity/basicity and solute-induced methanol O-H infrared frequency shifts. <i>Canadian Journal of Chemistry</i> , 1995, 73, 483-488.	0.6	164
120	Statistically-based interaction indices derived from molecular surface electrostatic potentials: a general interaction properties function (GIPF). <i>Computational and Theoretical Chemistry</i> , 1994, 307, 55-64.	1.5	183
121	Molecular surface electrostatic potentials and local ionization energies of Group V-VII hydrides and their anions: Relationships for aqueous and gas-phase acidities. <i>International Journal of Quantum Chemistry</i> , 1993, 48, 73-88.	1.0	146
122	Some proposed criteria for simulants in supercritical systems. <i>Computational and Theoretical Chemistry</i> , 1993, 281, 107-111.	1.5	12
123	Relationships between solute molecular properties and solubility in supercritical carbon dioxide. <i>The Journal of Physical Chemistry</i> , 1993, 97, 729-732.	2.9	48
124	Relationships of critical constants and boiling points to computed molecular surface properties. <i>The Journal of Physical Chemistry</i> , 1993, 97, 9369-9373.	2.9	81
125	Octanol/water partition coefficients expressed in terms of solute molecular surface areas and electrostatic potentials. <i>Journal of Organic Chemistry</i> , 1993, 58, 7070-7073.	1.7	69
126	Relationships between computed molecular properties and solute-solvent interactions in supercritical solutions. <i>The Journal of Physical Chemistry</i> , 1993, 97, 5144-5148.	2.9	38

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127	Polarizability and volume. <i>Journal of Chemical Physics</i> , 1993, 98, 4305-4306.	1.2	216
128	Partition coefficients of nitroaromatics expressed in terms of their molecular surface areas and electrostatic potentials. <i>The Journal of Physical Chemistry</i> , 1993, 97, 13807-13809.	2.9	31
129	A computational analysis of the bonding in boron trifluoride and boron trichloride and their complexes with ammonia. <i>Inorganic Chemistry</i> , 1993, 32, 2622-2625.	1.9	94
130	Calculated electrostatic potentials and local surface ionization energies of para-substituted anilines as measures of substituent effects. <i>Canadian Journal of Chemistry</i> , 1992, 70, 2209-2214.	0.6	66
131	Surface electrostatic potentials of halogenated methanes as indicators of directional intermolecular interactions. <i>International Journal of Quantum Chemistry</i> , 1992, 44, 57-64.	1.0	370
132	Quantitative determination of the total local polarity (charge separation) in molecules. <i>Molecular Physics</i> , 1992, 76, 609-617.	0.8	118
133	Investigation of relationships between solute molecule surface electrostatic potentials and solubilities in supercritical fluids. <i>The Journal of Physical Chemistry</i> , 1992, 96, 7938-7943.	2.9	62
134	Applications of calculated local surface ionization energies to chemical reactivity. <i>Computational and Theoretical Chemistry</i> , 1992, 255, 271-281.	1.5	62
135	Correlations between molecular electrostatic potentials and some experimentally-based indices of reactivity. <i>Computational and Theoretical Chemistry</i> , 1992, 256, 29-45.	1.5	114
136	Electrostatic potentials on the molecular surfaces of cyclic ureides. <i>The Journal of Physical Chemistry</i> , 1991, 95, 844-848.	2.9	49
137	Relationships between the aqueous acidities of some carbon, oxygen, and nitrogen acids and the calculated surface local ionization energies of their conjugate bases. <i>Journal of Organic Chemistry</i> , 1991, 56, 5012-5015.	1.7	74
138	A relationship between experimentally determined pK _a s and molecular surface ionization energies for some azines and azoles. <i>Journal of Organic Chemistry</i> , 1991, 56, 2934-2936.	1.7	68
139	Surface local ionization energies and electrostatic potentials of the conjugate bases of a series of cyclic hydrocarbons in relation to their aqueous acidities. <i>International Journal of Quantum Chemistry</i> , 1991, 40, 91-98.	1.0	25
140	Radial behavior of the average local ionization energies of atoms. <i>Journal of Chemical Physics</i> , 1991, 95, 6699-6704.	1.2	88
141	The use of the electrostatic potential at the molecular surface in recognition interactions: Dibenzo-p-dioxins and related systems. <i>Journal of Molecular Graphics</i> , 1990, 8, 81-85.	1.7	37
142	Average local ionization energies on the molecular surfaces of aromatic systems as guides to chemical reactivity. <i>Canadian Journal of Chemistry</i> , 1990, 68, 1440-1443.	0.6	363